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16. ABSTRACT

Multimedia exposure assessment models are being developed for the U.S. Environmental Protection Agency. Models are comprised of an atmospheric transport, degradation, dispersion and deposition module; a surface runoff module; and a surface water quality module. The modules are linked to describe theeffect of airborne, land based, and water bourne toxic organic pollutants on surface water quality. The data required for the air module include such input parameters as the settling velocity, deposition velocity, washout ratio and Henry's Law constant for the specific chemical being considered as well as the usual meteorological data for the particular area being modled. The surface runoff module will require data on the various physical watershed characteristics, which are related to topography, soil characteristics, land surface conditions, land use, etc. Individual storm hydrographs will also be required. The surface water quality module will need to simulate equilibrium partitioning of the toxic organic between dissolved, sediment adsorbed, or biomass adsorbed phases. Volitilization, hydrolysis, microbial transformation, photolysis, and oxidation need to be simulated. Environmental characterization of the surface water body would be required as well as the appropriate transformation rate constants and partition coefficients for the chemical being simulated.

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MULTIMEDIA EXPOSURE ASSESSMENT MODEL DATA NEEDS

by

Kenneth F. Hedden*

INTRODUCTION

Under the Toxic Substances Control Act (TSCA) chemicals must be evaluated for a potential hazard to human health or to the environment before they are marketed. An essential part of these evaluations is exposure assessment, the use of mathematical models that estimate the transport and transformations of potentially toxic substances in the environment. An exposure assessment should provide an estimate of the amount of a chemical to which an organism is exposed. Studies of toxicity in the laboratory and epidemilogical studies will allow an estimate of the health effects of a given amount of that chemical. Taken together this information will allow an assessment of risk to be made.

Any model for use in exposure assessment must address all potential routes of exposure, i.e., air, land, and water. Figure 1 illustrates the interrelationships of these exposure routes to man.

A number of mathematical models have been developed that describe each of the single media (2-4, 6, 7). In most ways the data needs of a multimedia model will be the sum of the needs of the individual models making up that multimedia model, but further constrained by the individual component model temporal and spatial characteristics.

Because models must be applied to potentially toxic substances not yet sold on the open market, no field data will be available. Consequently, methods must be available for determining parameters describing the rates of transformation and transport of a chemical through the environmental system in question. These parameters will be dependent on properties of the specific chemical in question as well as of the environment in which we are interested.

The purpose of this paper is to discuss the data needed for use in an exposure assessment model, i.e., a simulation technique that integrates mathematical descriptions of transport and

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transformation occurring through air, land runoff, and water routes. The data needs for such a multimedia exposure assessment model are initially addressed for each medium.

DATA REQUIREMENTS FOR MODELING AIR ENVIRONMENTS

Any air model used for multimedia exposure assessment must be consistent with the land runoff and water the models in level of approximation, in the classes of chemicals that can be described, and in resolution-- both temporal and spatial. The interface between the models will be by air-to-surface transfer of chemical. Calculation methods are available to estimate concentrations in air and air to surface transfer by wet- and dry-deposition (3,6). Input information includes meteorology data (such as wind speeds, wind directions, atmospheric stability, and hourly precipitation), source emissions inventories (to include information such as geographic locations, type and strength of emission source, height of stack, and plume rise factor), and material properties of the substance modeled (such as type of material, vapor pressure, solubility, particle size, and density). Outputs of the model are air concentrations of chemical as functions of time and location along with the fluxes of chemical from the atmosphere to the soil or water.

Source inventories generally include inputs from anthropogenic sources rather than contributions from distributed volatilization from water and soil. If the quantity of emissions from natural sources are significant and are susceptible to independent

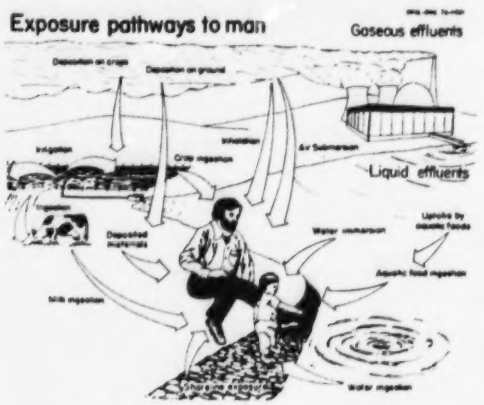

FIG. 1 EXPOSURE PATHWAYS TO MAN (Adapted from reference 4, courtesy of Oak Ridge National Laboratory, Health and Safety Research Division).

estimation, they can be incorporated in the same way as the anthropogenic sources. This approach avoids the need to run air, runoff, and aquatic models simultaneously. Coupling within a watershed defined by the aquatic and runoff models is from the air to the surface; significant coupling in the reverse direction does not occur because the residence time of air over the watershed is very short compared with that associated with the movement of water or soil within the watershed.

Gaussian dispersion formulations and first-order chemical degradation are appropriate assumptions for the air model. Various forms of the continuous source Gaussian models will normally be used based on source geometry, receptor geometry, and source/receptor distance. Transfer processes of fallout, dry deposition, and washout should be included.

The three classes of data normally required to run most air models are discussed in more detail below.

Meteorological Data

Meteorological data required consists of hourly wind speed, wind direction, and stability class. These data are available for major airports from the National Weather Service in Ashville, NC, and are preferred over STAR stability wind roses, which provide only joint frequency information. To run a model in an hourly sequential basis, it is necessary to have stability information (supplied or estimated) for each set of hourly wind speed observations. Stability information can be estimated from tables (9) using information on the cloud cover, which is ordinarily specified on a scale of 0-8 in the data sheets from the hourly weather observations.

Source Emission Data

Source emission rates for the primary pollutants (particulates, CO, SO_2, NO_x, and hydrocarbons) can be developed from from the National Emissions Data System in Research Triangle Park, NC,. If the pollutant of interest is associated with certain processes in the industrial classifications covered by the primary pollutant standards, it may be possible to estimate a scale factor relating the output of the pollutant of interest to one of the primary pollutant emission rates (10). In any event, fate assessment of pollutants in the environment must start from a material input schedule that relates the release of the toxic substance to certain anthropogenic or natural processes. To be on a consistent time basis with the meteorological observations, emissions data should be specified on an hourly basis. If the material is released from an elevated source, the plume height (H) must be estimated. For non-buoyant material emitted from the elevated source, this plume height is simply the source elevation; however, for buoyant plumes, some estimate of plume rise must be added to the source height in order to specify H (9).

Pollutant Properties

The pollutant attributes of interest range from broad categorization of properties, such as gaseous versus particulate and reactive versus non-reactive, to specific material properties, such as vapor pressure and solubility. If the material is in particulate form, measurement of the effective particle diameter will be required along with the particle density in order to calculate settling velocities. The solubility in water and vapor pressure of gaseous pollutants is needed in order to estimate the Henry's Law constant. Another set of material properties involves the chemical rate constants for hydroperoxyl radical and ozone attack in the atmosphere. Direct photolysis rates may also be necessary. Chemical rate constants are now becoming available in the literature (1).

DATA REQUIREMENTS FOR MODELING WATERSHED RUNOFF

Data requirements for a land runoff model may include information related to model operation, parameter evaluation, and model calibration (2,4). These requirements and possible sources of data are briefly discussed below.

Model Operation Data

The basic data for model operation are the input meteorologic data series. Normal operation may require hourly precipitation, daily potential evapotranspiration, and daily maximum and minimum air temperature. The period of record needed for each of these data series corresponds to the length of time for which simulation is performed. To minimize the impact of initial hydrologic conditions, a minimum of one year should normally be simulated. The actual time period of simulation depends on the information needed and the type of analysis being performed.

Parameter Evaluation Data

Data for runoff model parameter evaluation are obtained largely from physical watershed characteristics. These data include parameters that describe topography, soil characteristics, land surface conditions, hydrologic characteristics, climate, land use, etc. In general, the types of information needed for parameter evaluation include:

topographic maps
soil maps and investigations
hydrologic and meteorologic studies
water quality studies
land use maps and studies

Results of investigations related to the above topics for the watershed to be simulated should be collected and analyzed as a source of information for parameter evaluation.

Calibration Data

Many runoff models require calibration (2). Calibration involves the adjustment of parameters to improve agreement between recorded and simulated information. Observed runoff and water quality data are required. Ideally, the observed data should be continuous to allow an accurate assessment of the continuous simulation produced by the model. In addition, the continuous data should extend for three years to obtain an adequate calibration of the parameters. Data availability on most watersheds seldom is complete, however, especially for water quality. In such circumstances, calibration is limited to comparisons with whatever data can be obtained.

Hydrologic calibration involves comparison of simulated and recorded runoff volumes and individual storm hydrographs for a calibration period of one to three years. The volume comparison can be made on an individual storm or on a daily, monthly, or yearly basis depending on the watershed area, the length of the calibration period, and the available data. Minor storms with durations less than 15 minutes do not provide sufficient hydrograph definition for a valid comparison. Thus, data for hydrologic calibration must include both continuous runoff volumes and selected storm hydrographs throughout the calibration period.

Water quality calibration for nonpoint pollution is analogous to hydrologic calibration. Simulated pollutant mass removal comparisons to recorded data can be made on an individual storm or on a daily, monthly, or yearly basis, or as individual storm-pollutant graphs for selected storms. Because nonpoint pollution data are scarce, calibration is often reduced to comparing with the simulated values grab-sample measurements or selected storm-pollutant graphs. Actual data requirements for water quality calibration are thus often reduced to obtaining water quality data available for the watershed. For a model that simulates nonpoint pollution in terms of sediment (2), information on sediment (or Total Solids) yield and on the relationship between the individual pollutants and sediment would be the most pertinent.

DATA REQUIREMENTS FOR MODELING AQUATIC ENVIRONMENTS

Aquatic fate and transport models estimate the probable concentrations and distributions of chemicals in aquatic systems resulting from continuous discharge of low concentrations of these chemicals from industrial waste and surface runoff (4, 6, 7). The model must also assess the relative importance of photolysis, hydrolysis, oxidation, volatilization, sorption, and biotransformation or other appropriate processes in the removal of selected chemicals from solution in natural freshwater systems. Transfer through food chains or transformation on sediments, must eventually be addressed as well.

Simplifying assumptions concerning the various possible environmental transport and transformation processes in aquatic

systems are required for many existing models. Most assume that the overall rate of disappearance of a polluant from solution is controlled only by the transformation and transport processes that can be studied separately in the laboratory and by the hydraulic processes of the particular aquatic system being assessed.

Data must be acquired for each physical, chemical, and biological process believed to be important in the aquatic system under study. The data are then integrated by an appropriate computer model. Models are now available to simulate streams, ponds, and stratified lakes by suitable combinations of compartments and hydrologic parameters.

In the simplest application of an aquatic model, all data on transport and transformation processes are put in the form of simple first-order relationships in which only the dissolved concentration of the chemical is a variable. Rate constants and reactive environmental intermediates are lumped together as constants typical of a specific water body. This simple and preliminary assessment provides a good method of evaluating the relative importance of different transformation and transport processes, thereby eliminating additional data collection on subordinate processes.

The input data required are of two general types, environmental parameters describing the water body under consideration and information on the specific chemicals.

Environmental Data Requirements

The U.S. Environmental Protection Agency is assembling a computerized data base that includes many of the environmental parameters which may be needed for a number of river basins (8). Table 1 lists those parameters for which information is being collected.

Chemical Specific Requirements

The chemical-specific transport and transformation processes commonly incorporated in an aquatic model are hydrolysis, photolysis, oxidation, biodegradation, and equilibrium partitioning by volatilizaton or sorption. The environmental parameters listed in Table 1 together with these chemical-specific parameters will then determine at what rate a given chemical will be transported and/or transformed. Estimation procedures (Personal Communication, W. J. Lyman, A. D. Little, Inc., Cambridge, MA) and laboratory protocols (5) have been developed for determination of these and other chemical-specific parameters.

CONCLUSION

The objective to complete multimedia exposure assessments for toxic chemicals in the important environmental compartments (air, land, water) can initially be met by integrating existing single media models. The data needs for such an approach, in addition to

TABLE 1

ENVIRONMENTAL DATA REQUIREMENTS

Rivers	Lakes
Monthly average stream velocity	Lake depth
Monthly average cross-sectional area	Lake area
Monthly average flow rate	Lake volume
Approximate bed slope	Wind velocity
Type of water body (e.g., tidal, upland, etc.)	Cloud cover
Length of reach	Spectral composite zenith light extinction coefficient
Description of bed material (amount organic)	
Monthly average temperature	Temperature profile
Monthly average pH	pH
Monthly average suspended sediment concentration (% organic and/or size distribution when available)	Suspended sediment concentration (% organic carbon content)
Monthly average dissolved oxygen concentration	Dissolved organic carbon concentration
Monthly average total bacteria concentration	Actually sorbing biomass concentration

source emission inventories, include those specific to each environment being modeled and to each chemical of interest. Specific environmental data include but are not limited to meteorological data, precipitation data, topographic data, soil characteristics, land surface conditions, stream flow rate, lake area, depth, and volume, pH, temperature, suspended sediment concentration, and biomass concentration. Specific chemical data of interest range from broad categorization of properties, such as gaseous versus particulate and reactive versus non-reactive, to specific material properties such as vapor pressure, water solubility, and sorption coefficient. Much of the environmental data is available from various government agencies such as the National Weather Service or the Environmental Protection Agency. Specific chemical data is available from a variety of industrial and government sources, or may need to be estimated or measured in the laboratory.

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